Quantum Critical Behavior of a Three-Dimensional Ising Spin Glass in a Transverse Magnetic Field

Muyu Guo,[1] R. N. Bhatt,[1] and David A. Huse[2]
[1]Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544
[2]AT&T Laboratories, Murray Hill, New Jersey 07974
(Received 21 March 1994)

We present results of a Monte Carlo simulation study of the zero-temperature quantum phase transition of a three-dimensional short-range spin-$\frac{1}{2}$ Ising spin glass, driven by a transverse magnetic field. This quantum transition is equivalent to the finite-temperature transition in the (3+1)-dimensional anisotropic classical random Ising model that is the path integral of the quantum system. The critical exponents are estimated using a finite-size scaling analysis. The uniform linear susceptibility is finite at the transition, while the nonlinear susceptibility diverges. The results are more consistent with conventional, rather than activated, dynamic scaling in the quantum system.

PACS numbers: 75.10.Nr, 05.30.−d, 75.40.Cx, 75.40.Mg

Spin glasses have been the subject of experimental and theoretical investigations for almost two decades [1]. In high spatial dimension, d, they undergo a phase transition from a paramagnetic phase at high temperature, T, to a spin-glass ordered phase at low T. The ordered phase has long-range magnetic order, but in a random pattern chosen by the details of the spin-spin interaction in that particular sample of spin glass. For dimensions below the lower critical dimension (which is near $d=3$ for classical Ising spin glasses [2,3]), the ordered phase is confined to $T=0$, being unstable to thermal fluctuations.

The transition from a spin-glass phase to a paramagnetic phase can alternatively occur at zero temperature due to increasing *quantum* fluctuations [4]. This $T=0$ quantum phase transition has been investigated recently for Ising spin glasses in one dimension [5,6], as well as with infinite-range interactions [7–9]. A number of novel features have been discovered: For example, one obtains divergent susceptibilities in the paramagnetic phase in the case of $d=1$, whereas no such behavior is seen in the infinite range case. Besides the obvious issue of what happens in finite dimensions $d>1$, with realistic (range-dependent) interactions between spins, such systems are also of experimental interest. Recent experiments [10] have found substantial changes in the spin-glass critical behavior of the dipolar Ising system $LiHo_xY_{1-x}F_4$ with increasing transverse magnetic field.

In this Letter, we present results of Monte Carlo simulations of the nearest neighbor Ising spin glass on a simple cubic ($d=3$) lattice in a transverse magnetic field, characterized by the Hamiltonian

$$H_{\mathrm{qm}}=-\sum_{\langle i,j\rangle}J_{ij}\sigma_i^z\sigma_j^z-\Gamma\sum_i\sigma_i^x\,, \qquad (1)$$

where σ_i^α is the α component of a spin-$\frac{1}{2}$ spin operator at site i, and the J_{ij} are nearest neighbor interactions chosen to be independent quenched Gaussian random variables with zero mean and unit variance. Application of a magnetic field, Γ, transverse to the Ising (z) axis causes mixing of the eigenstates of the z components of the spins. At $T=0$ this system exhibits a continuous phase transition from a spin-glass ordered phase at small transverse fields to a paramagnetic phase for sufficiently large transverse fields. We have studied the critical scaling behavior at this transition, finding results consistent with conventional dynamic scaling with dynamic critical exponent $z\cong 1.3$, as opposed to the activated dynamic scaling that applies for $d=1$. The uniform magnetic susceptibility is found to be finite at the transition, in contrast to both $d=1$ and $d=2$ where it diverges [6,11]. The other critical exponents are also estimated.

We use the Suzuki-Trotter [12] formalism to map the $T=0$ quantum mechanical problem given by the Hamiltonian above, into a classical statistical mechanical system in 3+1 dimensions with the Hamiltonian

$$H_{\mathrm{cl}}=-A\sum_{\langle i,j\rangle,\tau}J_{ij}S_i(\tau)-B\sum_{i,\tau}S_i(\tau)S_i(\tau+1)\,, \qquad (2)$$

where the $S_i(\tau)=\pm 1$ are now classical Ising spins, representing the z component of the quantum spins at imaginary time τ. To precisely reproduce the ground state of the above quantum Hamiltonian [Eq. (1)], the limits $B\to\infty$ and $A\to 0$ must be taken in the appropriate fashion [12]. However, the universal properties of the phase transition are the same for finite, positive A and B as in this limit for both $d=1$ and the infinite-range model. This should be true quite generally, since the universal properties (i.e., critical exponents and scaling functions) do not depend on the short-length-scale details of the model. Thus for computational convenience we have simulated the case $A=1$, $B=1$, with τ taking on only integer values. This (3+1)-dimensional classical system orders at low temperatures into a phase with spin-glass order in the three "spatial" directions and ferromagnetic order at each site in the imaginary time (τ) direction. This low-temperature ordered phase of the classical system (2) corresponds directly to the low-transverse-field ordered phase of the quantum system (1) at zero temperature. Increasing the temperature in the classical system is equivalent to increasing the transverse field in the quantum system, and leads to a phase transition to the paramagnetic phase. *In the following we will discuss the* *behavior of the classical system (2) as a function of its temperature; this corresponds directly to the behavior of the zero-temperature quantum system (1) as a function of the transverse field.*

It has been found in dealing with classical spin models that finite-size scaling affords the most economical way of obtaining the critical behavior of the infinite-size system [13]. However, unlike isotropic models where the scaling is done equally for all dimensions that are being scaled, our model is anisotropic, and therefore the "space" and "τ" directions will not scale in the same fashion. In fact, one expects that near the critical point the correlation length in the τ direction ξ_τ, scales as a power of the correlation length in the space directions, ξ, so that $\xi_\tau \sim \xi^z$, where z is the dynamical critical exponent for the quantum system. In the absence of any information about z, we had to study the behavior as a function of the temperature and two finite sizes, the spatial size, L, and the size L_τ in the imaginary time direction. Conventional dynamic scaling then says that dimensionless quantities should scale as functions of two variables: the scaled shape, L_τ/L^z, and the scaled size, L/ξ, where ξ is the spatial correlation length in the infinite system. We have used periodic boundary conditions in both the space and imaginary time directions. The number of independent samples simulated ranges from 1024 for $L=4$ and $L_\tau=6$ to 144 for $L=10$ and $L_\tau=20$, requiring up to 2.5×10^5 Monte Carlo steps for equilibration and measurement.

As has been demonstrated for classical spin glasses, a very useful quantity to measure to determine the critical exponents is the overlap between two independent copies ("replicas") of the same spin-glass sample:

$$q=\sum_\tau \sum_i S_i^1(\tau) S_i^2(\tau)/L^3 L_\tau . \tag{3}$$

Here the superscript on the spin indicates the replica. Each replica has the same bonds J_{ij}, but is simulated with independent random initial conditions and independent heat baths at the same T. From q one can construct a dimensionless spin-glass coupling constant [2]

$$g(L,L_\tau,T)=[3-\langle q^4\rangle/\langle q^2\rangle^2]_{\mathrm{av}}/2 , \tag{4}$$

where the angular brackets denote a thermal average for a given realization of the random couplings J_{ij}, while $[\cdots]_{\mathrm{av}}$ denotes an average over such realizations. In a disordered phase for samples large compared to the correlation lengths, the overlap is a sum of many independent random local overlaps, so has a Gaussian distribution around $q=0$ and g then vanishes. In the ordered phase the overlap (spin-glass order parameter) acquires a nonzero value. If there is only one magnetization pattern that the system is ordering into then the magnitude of the overlap does not fluctuate in the limit of a large system and $g=1$. Near the critical point, g crosses over between these limiting values and should scale as

$$g=\bar{g}(L/\xi, L_\tau/L^z) , \tag{5}$$

where $\bar{g}$ is a universal scaling function of its *two* variables. If we fix L and T, we find g has a maximum as a function of L_τ. This occurs because for finite L and large L_τ we have effectively a one-dimensional system which must have a finite correlation length along the τ direction and when L_τ exceeds this correlation length g scales to zero as argued above. On the other hand, for T near T_c, large L and small L_τ we effectively have a three-dimensional system, which is well above its transition, so again g scales to zero. [$T_c(L_\tau)$ decreases with decreasing L_τ, and we are only trying to locate and study the transition in the large L_τ limit of the (3+1)-dimensional system.] Using this maximum in g, we can readily locate T_c, since it is only at T_c where this maximum value of g is independent of L. This behavior of g is illustrated schematically at the top of Fig. 1. We have found this procedure to be superior to more conventional procedures such as looking for the power-law decay of correlation functions, because the latter are significantly corrupted by finite-size effects.

Using the procedure described above, we find $T_c \cong 4.3$ for our classical model. At T_c, $L/\xi=0$, so from Eq. (5), g then depends only on the scaled shape L_τ/L^z. We find that $z\cong1.3$ causes the data for $g(L,L_\tau,T=4.3)$ to collapse best onto a single scaling curve. The resulting scaling plot is shown in Fig. 1. (Note that the maximum in g is actually very near $L_\tau=L^z$.) If this critical point were to have activated rather than conventional dynamic scaling, one would expect the peaks in g to grow broader with increasing L, when plotted on a logarithmic scale as in

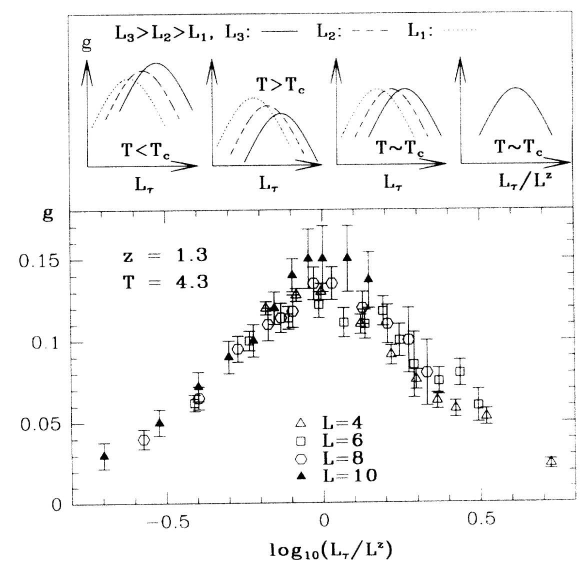

FIG. 1. Scaling of the coupling constant g [Eq. (4)] as sample size and shape are varied. Top plots schematically show the behavior below, at, and above T_c. The main graph shows the actual g, computed as a function of the scaled sample shape at T_c. The dynamic exponent $z\cong1.3$ and $T_c \cong 4.3$ are chosen for the best collapse of the data for different sizes onto one curve in this plot.

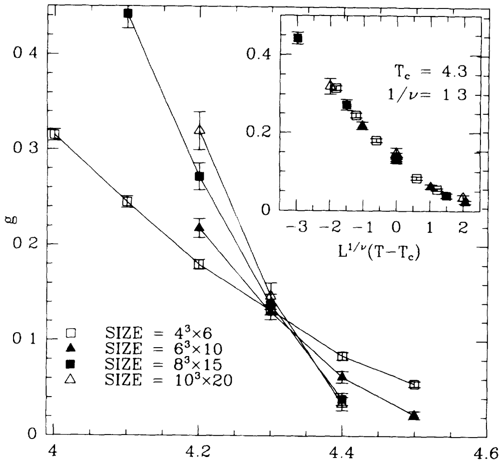

FIG. 2. The coupling constant, g, vs temperature for the scaled sample shape determined by the maximum of g in Fig. 1. The crossing indicates T_c. The inset shows the best collapse of these data onto one scaling curve.

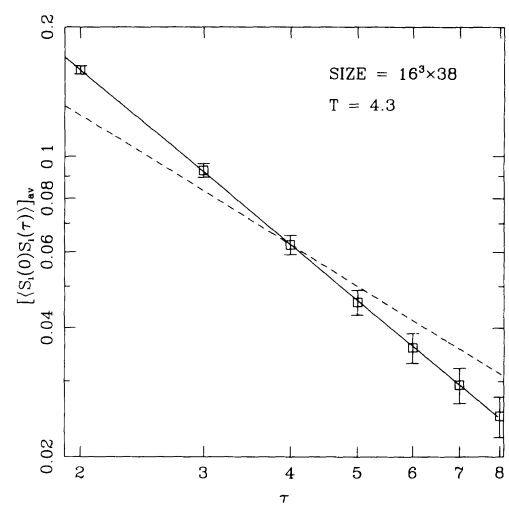

FIG. 3. Log-log plot of the imaginary time correlation function vs τ at the transition. The dashed line represents the power law $1/\tau$ on this plot. The autocorrelation function decays significantly faster than $1/\tau$, so its sum on τ, which is proportional to the uniform linear susceptibility [Eq. (6)], is finite.

Fig. 1. There is no sign of such a broadening, so we conclude that these data are more consistent with conventional, rather than activated, dynamic scaling.

Having determined z, we can fix the scaled shape and study the dependence of g on the scaled size L/ξ. We fix the scaled shape to be near the maximum of g vs L_τ in order to be insensitive to slight errors in our estimate of z, or to the rounding error because of the requirement that both L and L_τ are integers. The results for g vs T at each L are shown in Fig. 2. The intersection of the curves pinpoints the critical point T_c, which is seen to be close to 4.3 and is consistent with the earlier result from scaling of g. The inset in Fig. 2 is the scaling plot of the same data, with the temperature axis scaled, assuming, as usual, $\xi \sim |T-T_c|^{-\nu}$. The best collapse of the scaled data onto one curve occurs with correlation length exponent $1/\nu \cong 1.3$. Small systematic corrections to finite-size scaling can be seen in Figs. 1 and 2, in that the apparent T_c moves slightly higher when one examines larger samples [14]. Thus the true T_c may be somewhat higher than 4.3, and the effective exponents obtained from the length scales we study may differ a little from the true asymptotic critical exponents.

A striking result for the (1+1)-dimensional quantum Ising spin glass [6] is that the zero-temperature linear susceptibility to a uniform magnetic field oriented along the Ising axis is divergent due to Griffiths singularities in part of the paramagnetic phase, as well as at the critical point. For our (3+1)-dimensional system, on the other hand, this uniform linear susceptibility is finite even at the critical point. This susceptibility is proportional to

$$\chi_l = \sum_\tau [\langle S_i(0)S_i(\tau)\rangle]_{\rm av}, \tag{6}$$

and is hence finite if the average spin-spin correlation falls off with imaginary time faster than $1/\tau$. This correlation is shown in Fig. 3 for $T=4.3\cong T_c$. The decay is clearly faster than $1/\tau$; from $\tau=2$ to 8 the best fit is $\tau^{-1.3}$.

The nonlinear susceptibility is the divergent quantity at the transition that is experimentally accessible. It is proportional to the fourth cumulant of the total magnetization of the classical model:

$$\chi_{\rm nl} = [\langle M^4\rangle - 3\langle M^2\rangle^2]_{\rm av}/L^3L_\tau, \tag{7}$$

where $M=\sum_i\sum_\tau S_i(\tau)$. Noting that terms containing an odd number of spins at any given spatial site vanish after

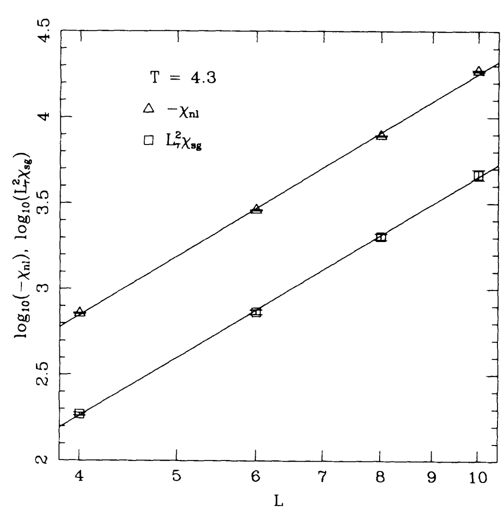

FIG. 4. Log-log plot of the nonlinear susceptibility and L_τ^2 times the spin-glass susceptibility vs sample size at the transition (for the "standard" scaled shapes used in Fig. 2). The slopes on this plot are identical, as expected from scaling, and equal to $2+2z-\eta \cong 3.5$.

doing the sample average, this expression becomes

$$\chi_{\rm nl} = \left[3\left\langle \left[\sum_i m_i^2\right]^2\right\rangle - 3\left[\sum_i \langle m_i^2\rangle\right]^2 - 2\sum_i \langle m_i^4\rangle + 6\sum_i \langle m_i^2\rangle^2 - 6\langle Q_m^2\rangle\right]_{\rm av} \Big/ L^3 L_\tau , \qquad (8)$$

where $m_i = \sum_\tau S_i(\tau)$ and $Q_m = \sum_i m_i^1 m_i^2$. The results of $\chi_{\rm nl}$ for $T = 4.3 \cong T_c$ are shown in Fig. 4. $\chi_{\rm nl}$ is expected to scale as

$$\chi_{\rm nl} \sim L^{2+2z-\eta} X(L/\xi, L_\tau/L^z) , \qquad (9)$$

where $X(x,y)$ is a scaling function. The results in Fig. 4 are for T_c at fixed scaled shape, so the slope on the log-log plot indicates $2+2z-\eta \cong 3.5$ or $\eta \cong 0.9$. Returning to the original quantum system (1), this scaling implies that if one sits at the critical transverse field, Γ_c, and varies the temperature (now of the quantum system), the nonlinear susceptibility diverges as one approaches this zero-temperature critical point as $\chi_{\rm nl} \sim T^{(\eta-2-2z)/z}$. The power-law exponent ($\cong 2.7$) is *close* to that obtained [13] for classical Ising spin glass ($\gamma \cong 2.9$). There are two possibilities for the dependence on the transverse field, Γ, near the critical point at $T=0$: If the Griffiths singularities are strong enough, $\chi_{\rm nl}$ is already divergent in the paramagnetic phase, as occurs in one dimension. If, on the other hand, $\chi_{\rm nl}$ is finite for Γ near but above Γ_c, then the critical divergence should be as $\chi_{\rm nl} \sim (\Gamma - \Gamma_c)^{\nu(\eta-2-2z)}$. We do not yet have a good estimate of the strength of the Griffiths singularities, except to say that they are weak enough that the uniform linear susceptibility remains finite.

We have also examined the "spin-glass susceptibility"

$$\chi_{\rm sg} = L^3 L_\tau [\langle q^2\rangle]_{\rm av} = \sum_j \sum_\tau [\langle S_i(0) S_j(\tau)\rangle^2]_{\rm av} . \qquad (10)$$

Since $\chi_{\rm sg}$ involves two fewer sums over τ than $\chi_{\rm nl}$, its expected scaling form is

$$\chi_{\rm sg} \sim L^{2-\eta} Y(L/\xi, L_\tau/L^z) . \qquad (11)$$

We have confirmed this scaling for our "standard" scaled shape at and near T_c. Figure 4 shows the results at T_c. For fixed scaled shape at T_c, scaling says that $\chi_{\rm nl}$ and $\chi_{\rm sg}$ should differ by a multiplicative factor proportional to L_τ^2. That this is true is demonstrated in Fig. 4, where the slopes on the log-log plot are indistinguishable.

In conclusion, we have studied the critical properties of the zero-temperature quantum phase transition of a three-dimensional short-range Ising spin-glass model, via a finite-size Monte Carlo simulation study of its classical counterpart. Our results are consistent with conventional dynamic scaling, with critical exponents $z \cong 1.3$, $1/\nu \cong 1.3$, and $\eta \cong 0.9$. The dynamic exponent is expected to be $z=2$ above the upper critical dimension [9], while it is infinite (activated dynamic scaling) for $d=1$ [6], so it is apparently nonmonotonic vs d. Our scaling results are very similar (albeit with somewhat different exponents, as expected) to those of Rieger and Young [11] who have been studying a two-dimensional system. The one difference is that the strong divergence of the uniform linear susceptibility that occurs for $d=1$ [6] is still present for $d=2$ [11] but is gone for $d=3$. We are currently studying the effects due to rare regions (Griffiths singularities) near the critical point in the disordered phase. A second issue requiring further investigation is the reason for the much weaker divergence of the nonlinear susceptibility seen in the experiments on $LiHo_xY_{1-x}F_4$.

We thank Heiko Rieger, Peter Young, Daniel Fisher, Nick Read, and Subir Sachdev for discussions. This work was supported in part by NSF Grants No. DMR-9224077 and No. CDA-9121709, and by DEC (DPRI). Computations were done on massively parallel MasPar computers at Princeton University and AT&T Bell Laboratories.

[1] K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986).
[2] R. N. Bhatt and A. P. Young, Phys. Rev. Lett. **54**, 924 (1985).
[3] A. T. Ogielski and I. Morgenstern, Phys. Rev. Lett. **54**, 928 (1985).
[4] A. J. Bray and M. A. Moore, J. Phys. C **13**, L655 (1980).
[5] R. Shankar and G. Murthy, Phys. Rev. B **36**, 536 (1987).
[6] D. S. Fisher, Phys. Rev. Lett. **69**, 534 (1992).
[7] Y. Goldschmidt and P.-Y. Lai, Phys. Rev. Lett. **64**, 2467 (1990).
[8] J. Miller and D. A. Huse, Phys. Rev. Lett. **70**, 3147 (1993).
[9] J. Ye, S. Sachdev, and N. Read, Phys. Rev. Lett. **70**, 4011 (1993).
[10] W. Wu, B. Ellman, T. F. Rosenbaum, G. Aeppli, and D. H. Reich, Phys. Rev. Lett. **67**, 2076 (1991); W. Wu *et al.*, *ibid.* **71**, 1919 (1993).
[11] H. Rieger and A. P. Young, following Letter, Phys. Rev. Lett. **72**, 4141 (1994).
[12] M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976).
[13] R. N. Bhatt and A. P. Young, *Heidelberg Colloquium on Glassy Dynamics* (Springer-Verlag, Berlin, 1987), p. 215.
[14] The same has been observed in classical spin glasses: see curves for the SK model in Ref. [2], and also R. N. Bhatt and A. P. Young, J. Magn. Magn. Mater. **54-57**, 191 (1986).